

# Effective $\mathbf{kp}$ -Hamiltonian and correct boundary conditions for envelope functions in $A_3B_5$ -heterostructures. Method of invariants.

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## Abstract

Method of invariants is used to obtain effective  $\mathbf{kp}$ -Hamiltonian with position-dependent band parameters and correct boundary conditions for electron and hole envelope functions in  $A_3B_5$ -heterostructures with arbitrary interface orientation. It is shown that the presence of heterointerface yields additional quadratic-in- $\mathbf{k}$  and linear-in- $\mathbf{k}$  terms in the kinetic energy operator of electron and hole due to non-commutativity of position-dependent band parameters and momentum operator. In particular, the  $\Gamma_6$  conduction band Hamiltonian is determined by two position-dependent band parameters:  $\alpha_1 = m_0/m_e$  and additional parameter  $\alpha_2$ . Similarly for description of the  $\Gamma_8$  valence band  $\mathbf{kp}$ -Hamiltonian the three Luttinger parameters  $\gamma_1$ ,  $\gamma_2$  and  $\gamma_3$  are no longer sufficient, and introducing of two additional parameters  $\gamma_4$  and  $\gamma_5$ , that determine quadratic-in- $\mathbf{k}$  terms, and additional parameter  $\beta_1$ , determining a linear-in- $\mathbf{k}$  term, is necessary. The additional terms in the  $\Gamma_6$  and  $\Gamma_8$   $\mathbf{kp}$ -Hamiltonians, which are proportional to  $\alpha_2$  and  $\gamma_4$ ,  $\gamma_5$ , appear due to interaction at the interface of electron spin and hole effective spin with their orbital motion, which is described by envelope functions (interface effective spin-orbit interaction). The parameters  $\alpha_2$  and  $\gamma_5$  arise due to relativistic effects and appear in the second order of  $\mathbf{kp}$ -perturbation theory only when spin-orbit splitting of intermediate states is taken into account. The parameter  $\gamma_4$  is non-relativistic and can be approximately related to the Luttinger parameters as  $\gamma_4 = (1/3)(-1 - \gamma_1 + 2\gamma_2 + 3\gamma_3)$ . The additional linear-in- $\mathbf{k}$  term, which is determined by the parameter  $\beta_1$ , is also non-relativistic and arises due to variation of the Bloch functions across the interface. In the framework of this approach the  $\Gamma_8 \oplus \Gamma_7$  valence band  $\mathbf{kp}$ -Hamiltonian is derived. Presence of heterointerface gives rise to short range interface  $\delta$ -corrections, which are also determined by the method of invariants. The new form of the Hamiltonian allows us to obtain the correct boundary conditions for envelope functions of electron and hole in  $A_3B_5$ -heterostructures with arbitrary orientated heterointerface.

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## I. INTRODUCTION

In spite of the fact that the effective-mass theory for semiconductor heterostructures was being widely discussed in the literature [1]-[8], by now there is no unified opinion about the proper form of **kp**-Hamiltonian and corresponding boundary conditions for electron and hole envelope functions [9]-[12]. In the present work it is shown that similarly to the case of bulk material the effective mass Hamiltonian in a system with heterointerface can be determined in the framework of **kp**-perturbation theory by means of the finite number of band parameters. However, due to absence of a translational symmetry these parameters become position-dependent and, generally, their number exceeds the number of similar parameters in the bulk material [13]. Besides that the presence of interface gives rise to additional short range interface  $\delta$ -corrections, which are, in particular, responsible for mixing of light and heavy hole states in the  $\Gamma_8$  valence band [14]. The approach used in this paper is close to the one used by Karavaev and Tikhodeev [3] and by Foreman [8], [10].

Using the method of invariants we have shown that in contrast to the bulk material in a heterointerface system the kinetic energy operator of electron in the  $\Gamma_6$  band up to quadratic-in- $\mathbf{k}$  terms is determined by two position-dependent parameters  $\alpha_1$  and  $\alpha_2$ . The first one is the inverse effective mass of electron in the  $\Gamma_6$  band:  $\alpha_1 = m_o/m_e$ . The second  $\alpha_2$  is an additional parameter that determines a correction to the effective Hamiltonian which is responsible for electron spin-orbit interaction at the interface, calculated by means of envelope functions. It arises in the second order of **kp**-perturbation theory when spin-orbit splitting of intermediate states is taken into account. Neglecting **kp**-interaction of the  $\Gamma_6(\Gamma_1^c)$  conduction band with all other states, except the nearest  $\Gamma_8 \oplus \Gamma_7(\Gamma_{15}^v)$  valence band, this relativistic parameter is proportional to the  $\Gamma_{15}^v$  valence band spin-orbit splitting  $\Delta_{so}$ :  $\alpha_2 = [\Delta_{so}/(3E_g + 2\Delta_{so})](1 - m_o/m_e)$ , where  $E_g = E_c^{\Gamma_6} - E_v^{\Gamma_8}$ ,  $\Delta_{so} = E_v^{\Gamma_8} - E_v^{\Gamma_7}$ .

Similarly it is shown that the hole kinetic energy operator in the  $\Gamma_8$  band up to the second power of  $\mathbf{k}$  accuracy (excluding linear relativistic terms) is determined by six position-dependent parameters. Three of them  $\gamma_1$ ,  $\gamma_2$  and  $\gamma_3$  coincide with the usual Luttinger parameters for the bulk material, the three additional ones  $\gamma_4$ ,  $\gamma_5$  and  $\beta_1$  arise due to the presence of heterointerface. The additional quadratic-in- $\mathbf{k}$  terms in the  $\Gamma_8$  band **kp**-Hamiltonian, which are proportional to  $\gamma_4$  and  $\gamma_5$ , appear due to interaction of hole effective spin ( $J = 3/2$ ) with its orbital momentum at the interface, calculated by means of smooth envelope functions. The relativistic parameter  $\gamma_5$  is analogous to the parameter  $\alpha_2$  of the  $\Gamma_6$  band and if we take into account interaction of the  $\Gamma_8(\Gamma_{15}^v)$  valence band only with the nearest  $\Gamma_8 \oplus \Gamma_7(\Gamma_{15}^c)$  conduction band it is proportional to the spin-orbit splitting  $\Delta'_{so}$  of the  $\Gamma_{15}^c$  conduction band:  $\gamma_5 = (1/18)(1 + \gamma_1 - 2\gamma_2) [\Delta'_{so}/(E'_g + \Delta'_{so})]$ , where  $E'_g = E_c^{\Gamma_7} - E_v^{\Gamma_8}$ ,  $\Delta'_{so} = E_c^{\Gamma_8} - E_c^{\Gamma_7}$ . The non-relativistic parameter  $\gamma_4$  can be approximately related to the Luttinger parameters as:  $\gamma_4 = (1/3)(-1 - \gamma_1 + 2\gamma_2 + 3\gamma_3)$ . The parameter  $\beta_1$  determines an additional linear-in- $\mathbf{k}$

non-relativistic term and arises due to variation of the Bloch functions across interface.

The additional quadratic-in- $\mathbf{k}$  terms in the  $\Gamma_6$  and  $\Gamma_8$  **kp**-Hamiltonians, that are proportional to the parameters  $\alpha_2$  and  $\gamma_4, \gamma_5$ , which are absent in the bulk material, take place only in the non-homogenous systems with disturbed translational symmetry. These terms describe interaction of electron spin and hole effective spin with their orbital momentum, calculated by means of smooth envelope functions, in the narrow interface region. This interface effective spin-orbit interaction takes place in the  $\Gamma_{15}$  valence band, where the hole should be attributed effective spin  $J = 1$ . It explains non-relativistic background of the parameter  $\gamma_4$  in the  $\Gamma_8$  **kp**-Hamiltonian.

This approach was used to obtain the hole  $\Gamma_8 \oplus \Gamma_7(\Gamma_{15}^v)$  two-band **kp**-Hamiltonian in heterosystem. It was shown that if we consider the  $\Gamma_8 \oplus \Gamma_7$  valence band states as formed exclusively by the  $\Gamma_{15}^v$  state, i.e. neglecting spin-orbit mixing of these states with other states, quadratic-in- $\mathbf{k}$  terms of the  $6 \times 6$  hole **kp**-Hamiltonian are determined by five position-dependent parameters  $\gamma_1, \gamma_2, \gamma_3$  and  $\gamma_4$ . Besides that the  $\Gamma_8 \oplus \Gamma_7$  valence band **kp**-Hamiltonian includes a non-relativistic linear-in- $\mathbf{k}$  term proportional to the parameter  $\beta_1$  of the  $\Gamma_8$  band.

Taking into account short range part of the interface potential gives rise to additional interface short range  $\delta$ -corrections in the effective mass Hamiltonian, which also include  $\mathbf{k}$ -dependent terms. These corrections modify boundary conditions for envelope functions and their derivatives and lead to additional spin-dependent effects of electron and hole interface scattering. Using the method of invariants we can determine the form of these corrections for the case of arbitrary orientated heterointerface.

The effective **kp**-Hamiltonians obtained in this paper allow us to derive the correct boundary conditions for electron and hole envelope functions in  $A_3B_5$ -heterostructures with arbitrary orientated heterointerface. As an example we obtained boundary conditions for heterostructure with (001) interface.

## II. EFFECTIVE MASS APPROXIMATION IN HETEROINTERFACE SYSTEM. POSITION-DEPENDENT PSEUDO-COORDINATE BASIS

In contrast to the bulk material, a system with heterointerface does not have a translational symmetry and therefore electron wave vector  $\mathbf{k}$  is not a good quantum number any more. The electron and hole scattering processes at the heterointerface, changing the wave vector from  $\mathbf{k}$  to  $\mathbf{k}'$ , lead to the fact that **kp**-Hamiltonian of the heterosystem becomes dependent on two variables  $\mathbf{k}$  and  $\mathbf{k}'$ .

Let's represent the Hamiltonian of a system with heterointerface in the following form:

$$H = \frac{\mathbf{p}^2}{2m_0} + U_1(\mathbf{x}) + f(\mathbf{x}) \cdot \Delta U(\mathbf{x}). \quad (1)$$

Here  $U_{1,2}(\mathbf{x})$  are the crystal potentials on the left and right sides of the interface respectively, which have the same period and symmetry;  $\Delta U(\mathbf{x}) = U_2(\mathbf{x}) - U_1(\mathbf{x})$ ;  $f(\mathbf{x}) \equiv f(\mathbf{n}\mathbf{x})$  is a step-like function, which modulates periodic potential in the direction perpendicular to the interface;  $\mathbf{n}$  is a unit vector which is normal to the interface. Usually to solve Schrödinger equation with the Hamiltonian (1), the Kohn-Luttinger basis  $|\alpha, n, \mathbf{k}\rangle = e^{i\mathbf{k}\mathbf{x}} |\alpha, n\rangle$  is used, where  $|\alpha, n\rangle$  is a Bloch state at  $\mathbf{k} = 0$ , satisfying the Schrödinger equation for the bulk crystal with periodic potential  $U_1(\mathbf{x})$

$$\left[ \frac{\mathbf{p}^2}{2m_0} + U_1(\mathbf{x}) \right] |\alpha, n\rangle = E^{(\alpha)} |\alpha, n\rangle,$$

where  $\alpha$  labels bands (including irreducible representations) at the  $\Gamma$  point of Brillouin zone, and  $n$  refers to degenerate states (partners). In the Kohn-Luttinger basis the Hamiltonian (1) has the following form:

$$\begin{aligned} \langle \alpha, n, \mathbf{k} | H | \alpha', n', \mathbf{k}' \rangle = & \left( E^{(\alpha)} + \frac{\hbar^2 k^2}{2m_0} \right) \delta_{\alpha\alpha'} \delta_{nn'} \delta_{\mathbf{k}\mathbf{k}'} + \\ & f(\mathbf{k} - \mathbf{k}') \Delta U^{\alpha\alpha'} \delta_{nn'} + \frac{\hbar}{m_0} \mathbf{k} \mathbf{p}_{nn'}^{\alpha\alpha'} \delta_{\mathbf{k}\mathbf{k}'} + V_{nn'}^{\alpha\alpha'}(\mathbf{k} - \mathbf{k}'), \end{aligned} \quad (2)$$

where  $f(\mathbf{k} - \mathbf{k}') = f(k_\perp - k'_\perp) \delta_{\mathbf{k}_\parallel \mathbf{k}'_\parallel}$  is a Fourier transformant of  $f(\mathbf{x})$ ,  $k_\perp = \mathbf{n}\mathbf{k}$ ,  $\mathbf{k}_\parallel = \mathbf{k} - \mathbf{n}k_\perp$ ;  $\mathbf{p}_{nn'}^{\alpha\alpha'} = \langle \alpha, n | \mathbf{p} | \alpha', n' \rangle$ ;  $\Delta U^{\alpha\alpha'} \delta_{nn'} = \Delta U_{nn'}^{\alpha\alpha'}(0)$  are matrix elements which determine smooth part of the interface scattering potential and couple states of the same symmetry;  $V_{nn'}^{\alpha\alpha'}(\mathbf{k} - \mathbf{k}') = V_{nn'}^{\alpha\alpha'} \delta_{\mathbf{k}_\parallel \mathbf{k}'_\parallel}$  are interface short range corrections;  $V_{nn'}^{\alpha\alpha'} = \sum_{G_\perp \neq 0} f(G_\perp) \Delta U_{nn'}^{\alpha\alpha'}(G_\perp, \mathbf{G}_\parallel = 0)$ ;  $\Delta U_{nn'}^{\alpha\alpha'}(\mathbf{G}) = (1/\Omega) \int_\Omega u_{n0}^{\alpha*}(\mathbf{x}) \Delta U(\mathbf{x}) u_{n'0}^{\alpha'}(\mathbf{x}) e^{i\mathbf{G}\mathbf{x}} d\mathbf{x}$ ;  $\mathbf{G}$  is the reciprocal lattice vector,  $G_\perp = \mathbf{n}\mathbf{G}$ ,  $\mathbf{G}_\parallel = \mathbf{G} - \mathbf{n}G_\perp$ ;  $(1/\sqrt{V})u_{n0}^\alpha(\mathbf{x}) = \langle \mathbf{x} | \alpha, n \rangle$  are Bloch wave functions at  $\mathbf{k} = 0$ ,  $V$  is the crystal volume,  $\Omega$  is the primitive cell volume.

To apply the effective mass approximation to heterointerface systems it is convenient to use pseudo-Wannier basis  $|\alpha, n, \mathbf{R}_m\rangle$ , which is related to the Kohn-Luttinger basis  $|\alpha, n, \mathbf{k}\rangle$  by a unitary transformation

$$|\alpha, n, \mathbf{R}_m\rangle = \sqrt{\frac{\Omega}{V}} \sum_{\mathbf{k}}^{BZ} |\alpha, n, \mathbf{k}\rangle e^{-i\mathbf{k}\mathbf{R}_m}, \quad (3)$$

where  $\mathbf{R}_m$  are discrete Bravais lattice vectors and the summation is performed over Brillouin zone. This basis satisfies the conditions of orthonormality and completeness

$$\langle \alpha, n, \mathbf{R}_m | \alpha', n', \mathbf{R}_{m'} \rangle = \delta_{\alpha\alpha'} \delta_{nn'} \delta_{\mathbf{R}_m \mathbf{R}_{m'}},$$

$$\sum_{\alpha, n, \mathbf{R}_m} |\alpha, n, \mathbf{R}_m\rangle \langle \alpha, n, \mathbf{R}_m| = 1.$$

In the framework of the effective mass approximation it is assumed that the envelope wave functions  $\psi_n^\alpha(\mathbf{k}) = \langle \alpha, n, \mathbf{k} | \psi \rangle$  and matrix elements of the Hamiltonian (2) (excluding the short-range part) are localized in a small area of  $\mathbf{k}$ -space inside of the Brillouin zone and the summation in (3) can be extended to the whole infinite  $\mathbf{k}$ -space. In this approximation we can consider  $\mathbf{R}_m$  as a continuous variable  $\mathbf{R}$  and the pseudo-Wannier basis transforms into pseudo-coordinate basis

$$|\alpha, n, \mathbf{R}\rangle = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} |\alpha, n, \mathbf{k}\rangle e^{-i\mathbf{k}\mathbf{R}}, \quad (4)$$

which satisfies the following conditions of orthonormality and completeness:

$$\begin{aligned} \langle \alpha, n, \mathbf{R} | \alpha', n', \mathbf{R}' \rangle &= \delta_{\alpha\alpha'} \delta_{nn'} \delta(\mathbf{R} - \mathbf{R}'), \\ \sum_{\alpha, n} \int d\mathbf{R} |\alpha, n, \mathbf{R}\rangle \langle \alpha, n, \mathbf{R}| &= 1. \end{aligned} \quad (5)$$

The Hamiltonian (1) in this basis according to (2), (4) and (5) has the following form:

$$\begin{aligned} \langle \alpha, n, \mathbf{R} | H | \alpha', n', \mathbf{R}' \rangle &= \frac{1}{V} \sum_{\mathbf{k}, \mathbf{k}'} e^{i\mathbf{k}\mathbf{R}} \langle \alpha, n, \mathbf{k} | H | \alpha', n', \mathbf{k}' \rangle e^{-i\mathbf{k}'\mathbf{R}'} = \\ &= \left[ E^{(\alpha)} \delta_{\alpha\alpha'} + \tilde{f}(\mathbf{R}) \Delta U^{\alpha\alpha'} \right] \delta_{nn'} \delta(\mathbf{R} - \mathbf{R}') - \frac{\hbar^2}{2m_0} [\nabla_{\mathbf{R}}^2 \delta(\mathbf{R} - \mathbf{R}')] \delta_{\alpha\alpha'} \delta_{nn'} + \\ &\quad \frac{\hbar}{m_0} [-i \nabla_{\mathbf{R}} \delta(\mathbf{R} - \mathbf{R}')] \mathbf{p}_{nn'}^{\alpha\alpha'} + V_{nn'}^{\alpha\alpha'}(\mathbf{R}) \delta(\mathbf{R} - \mathbf{R}'). \end{aligned} \quad (6)$$

Here  $\tilde{f}(\mathbf{R}) = \sum_{\mathbf{k}} f(\mathbf{k}) e^{i\mathbf{k}\mathbf{R}}$  is a smooth modulating function,  $V_{nn'}^{\alpha\alpha'}(\mathbf{R}) = \sum_{\mathbf{k}} V_{nn'}^{\alpha\alpha'}(\mathbf{k}) e^{i\mathbf{k}\mathbf{R}}$  are interface short range corrections. In the effective mass approximation we can consider  $\tilde{f}(\mathbf{R}) \approx \Theta(\mathbf{n}\mathbf{R})$  and  $V_{nn'}^{\alpha\alpha'}(\mathbf{R}) \approx \tilde{V}_{nn'}^{\alpha\alpha'} \delta(\mathbf{n}\mathbf{R})$ , where  $\Theta(\mathbf{n}\mathbf{R})$  and  $\delta(\mathbf{n}\mathbf{R})$  are one-dimensional step-function and  $\delta$ -function respectively.

The short range part of the Hamiltonian, characterized by matrix  $\tilde{V}_{nn'}^{\alpha\alpha'}$ , is determined by the nature of atoms constituting the heterointerface and their disposition. For ideal heterointerface the elements of this matrix can be, in principal, calculated by microscopic theory [14] - [17]. In the effective mass approximation symmetry of the short range corrections is determined exclusively by the symmetry of the crystal and orientation of the interface. Therefore it can be included into the Hamiltonian as an additional phenomenological term. Near to the interface plane, which is determined by the equation  $\mathbf{n}\mathbf{x} = 0$ , the short range part of the interface potential  $V^S(\mathbf{n}\mathbf{x})$  can be written in the form of the following decomposition:

$$V^S(\mathbf{n}\mathbf{x}) = V^S(0) + V^{S'}(0) \sum_i n_i x_i + \frac{1}{2} V^{S''}(0) \sum_{i,j} n_i n_j x_i x_j + \dots$$

The position of the interface is determined by the condition  $V^S(0) = 0$ . Therefore the first term in the right hand side of this decomposition can be omitted. The second term, which is proportional to  $V^{S'}(0)$ , characterizes magnitude of the uniform electric field localized in the interface region and is the most significant. The third and the following terms characterize non-uniformity of this field. Thus from the phenomenological standpoint the matrix of the short range interface correction  $\tilde{V}$  can be written as a decomposition in the powers of  $\mathbf{n}$

$$\tilde{V} = \sum_i \tilde{V}_i n_i + \frac{1}{2} \sum_{i,j} \tilde{V}_{ij} n_i n_j + \dots,$$

in which the most significant role plays the term proportional to  $\mathbf{n}$ .

The locality of the Hamiltonian (6) allows us, at every point of  $\mathbf{R}$ -space, to get rid of the off-diagonal matrix elements  $\tilde{f}(\mathbf{R})\Delta U^{\alpha\alpha'}$  which mix states of the same symmetry. To do that let us introduce a unitary matrix  $\mathbf{S}(\mathbf{R})$ , which at any point  $\mathbf{R}$  satisfies the conditions:  $\mathbf{S}^+(\mathbf{R})\mathbf{S}(\mathbf{R}) = \mathbf{1}$  ( $\mathbf{1}$  is a unit matrix), and diagonalizes smooth part of the potential energy operator of the Hamiltonian (6)

$$\sum_{\alpha'',\alpha'''} S^{+\alpha\alpha''}(\mathbf{R}) \left[ E^{(\alpha'')} \delta_{\alpha''\alpha'''} + \tilde{f}(\mathbf{R})\Delta U^{\alpha''\alpha'''} \right] S^{\alpha'''\alpha'}(\mathbf{R}) = E^{(\alpha)}(\mathbf{R}) \delta_{\alpha\alpha'}. \quad (7)$$

Here  $E^{(\alpha)}(\mathbf{R})$  is position-dependent energy of electron in  $\alpha$  band at  $\mathbf{k} = 0$ , which determines the band offset at the interface. Matrix elements  $S^{\alpha\alpha'}(\mathbf{R})$  are solutions of the following system of eigenvalue equations:

$$\sum_{\alpha'} \left[ E^{(\alpha)} \delta_{\alpha\alpha'} + \tilde{f}(\mathbf{R})\Delta U^{\alpha\alpha'} \right] S^{\alpha'\alpha''}(\mathbf{R}) = E^{(\alpha'')}(\mathbf{R}) S^{\alpha\alpha''}(\mathbf{R}),$$

where  $\mathbf{R}$  is a parameter.

Unitary transformation of the Hamiltonian (6) by the matrix  $\mathbf{S}(\mathbf{R})$  is equivalent to using a new position-dependent pseudo-coordinate basis

$$|S_n^\alpha, \mathbf{R}\rangle = \sum_{\alpha'} |\alpha', n, \mathbf{R}\rangle S^{\alpha'\alpha}(\mathbf{R}),$$

which in the effective mass approximation takes account of variation of the Bloch states at  $\mathbf{k} = 0$  across interface. The Schrödinger equation in this basis can be written as:

$$\sum_{\alpha', n'} \int d\mathbf{R}' \langle S_n^\alpha, \mathbf{R} | H | S_{n'}^{\alpha'}, \mathbf{R}' \rangle \langle S_{n'}^{\alpha'}, \mathbf{R}' | \psi \rangle = E \langle S_n^\alpha, \mathbf{R} | \psi \rangle, \quad (8)$$

where the Hamiltonian is

$$\langle S_n^\alpha, \mathbf{R} | H | S_{n'}^{\alpha'}, \mathbf{R}' \rangle = \sum_{\alpha'', \alpha'''} S^{+\alpha\alpha''}(\mathbf{R}) \langle \alpha'', n, \mathbf{R} | H | \alpha''', n', \mathbf{R}' \rangle S^{\alpha''' \alpha'}(\mathbf{R}'). \quad (9)$$

Transformation (9) does not break the locality of the Hamiltonian of the heterosystem and therefore the equation (8) is a differential equation and can be represented as:

$$\sum_{\alpha', n'} \left[ E^{(\alpha)}(\mathbf{R}) \delta_{\alpha\alpha'} \delta_{nn'} + T_{nn'}^{\alpha\alpha'}(\hat{\mathbf{k}}, \mathbf{R}) \right] \psi_{n'}^{\alpha'}(\mathbf{R}) = E \psi_n^\alpha(\mathbf{R}), \quad (10)$$

where

$$T_{nn'}^{\alpha\alpha'}(\hat{\mathbf{k}}, \mathbf{R}) = \sum_{\alpha'', \alpha'''} S^{+\alpha\alpha''}(\mathbf{R}) \left[ \frac{\hbar^2}{2m_0} \hat{\mathbf{k}}^2 \delta_{\alpha''\alpha'''} \delta_{nn'} + \frac{\hbar}{m_0} \hat{\mathbf{k}} \mathbf{p}_{nn'}^{\alpha''\alpha'''} + V_{nn'}^{\alpha''\alpha'''}(\mathbf{R}) \right] S^{\alpha''' \alpha'}(\mathbf{R})$$

and  $\hat{\mathbf{k}} = -i\partial/\partial\mathbf{R}$ ,  $\psi_n^\alpha(\mathbf{R}) = \langle S_n^\alpha, \mathbf{R} | \psi \rangle$ .

Renormalized single-band Hamiltonian  $H_{nn'}^{(\alpha)}(\hat{\mathbf{k}}, \mathbf{R})$  is obtained by excluding from the system of equations (10) all states  $\beta \neq \alpha$  [4]. Green's function  $G^{(\beta)}(E, \mathbf{R}) = 1/[E - E^{(\beta)}(\mathbf{R})]$ , which is usually used in this procedure, can be approximately substituted by  $G^{(\beta)}[E^\alpha(\mathbf{R}), \mathbf{R}] = 1/[E^\alpha(\mathbf{R}) - E^{(\beta)}(\mathbf{R})]$ . Up to the terms of the second order this corresponds to the standard perturbation theory. As a result we get

$$H_{nn'}^{(\alpha)}(\hat{\mathbf{k}}, \mathbf{R}) = E^{(\alpha)}(\mathbf{R}) \delta_{nn'} + T_{nn'}^{\alpha\alpha}(\hat{\mathbf{k}}, \mathbf{R}) + \sum_{\substack{\beta \neq \alpha, \\ m}} T_{nm}^{\alpha\beta}(\hat{\mathbf{k}}, \mathbf{R}) \frac{1}{E^{(\alpha)}(\mathbf{R}) - E^{(\beta)}(\mathbf{R})} T_{mn'}^{\beta\alpha}(\hat{\mathbf{k}}, \mathbf{R}) + \dots, \quad (11)$$

where omitted right hand side terms correspond to the corrections of the third and higher orders of the perturbation theory.

Commutation relations

$$\mathbf{S}^+(\mathbf{R}) \hat{\mathbf{k}} - \hat{\mathbf{k}} \mathbf{S}^+(\mathbf{R}) = i \partial \mathbf{S}^+(\mathbf{R}) / \partial \mathbf{R},$$

$$\mathbf{S}(\mathbf{R}) \hat{\mathbf{k}} - \hat{\mathbf{k}} \mathbf{S}(\mathbf{R}) = i \partial \mathbf{S}(\mathbf{R}) / \partial \mathbf{R},$$

allow us to transform the single-band  $\mathbf{k}\mathbf{p}$ -Hamiltonian (11) to the canonical form. The additional terms, containing  $\partial \mathbf{S}^+(\mathbf{R}) / \partial \mathbf{R}$  and  $\partial \mathbf{S}(\mathbf{R}) / \partial \mathbf{R} \sim \mathbf{n} \delta(\mathbf{n}\mathbf{R})$ , arise due to difference of the Bloch wave functions on the both sides of the interface and in the framework of the effective mass approximation can be attached to the short range  $\delta$ -corrections.

Taking into account all stated above the single-band Hamiltonian (11) can be written as a sum of two terms

$$H_{nn'}^{(\alpha)}(\hat{\mathbf{k}}, \mathbf{R}) = H_{nn'}^{0(\alpha)}(\hat{\mathbf{k}}, \mathbf{R}) + H_{nn'}^{S(\alpha)}(\hat{\mathbf{k}}, \mathbf{R}). \quad (12)$$

Here  $H_{nn'}^{0(\alpha)}(\hat{\mathbf{k}}, \mathbf{R})$  is a bulk-like part of  $\mathbf{k}\mathbf{p}$ -Hamiltonian which can be written up to the terms proportional to  $\hat{k}_i \hat{k}_j$  in the following form:

$$H_{nn'}^{0(\alpha)}(\hat{\mathbf{k}}, \mathbf{R}) = E^{(\alpha)}(\mathbf{R})\delta_{nn'} + \frac{1}{2} \frac{\hbar}{m_0} \left[ \hat{\mathbf{k}} \mathbf{p}_{nn'}^{(\alpha)}(\mathbf{R}) + \mathbf{p}_{nn'}^{(\alpha)}(\mathbf{R}) \hat{\mathbf{k}} \right] + \frac{\hbar^2}{2m_0} \hat{k}_i M_{nn'}^{(\alpha)}(\mathbf{R}) \hat{k}_j, \quad (13)$$

where

$$M_{nn'}^{(\alpha)}(\mathbf{R}) = \delta_{ij} \delta_{nn'} + \frac{2}{m_0} \sum_{\substack{\beta \neq \alpha, \\ m}} \frac{[\mathbf{p}_{nm}^{\alpha\beta}(\mathbf{R})]_i [\mathbf{p}_{mn'}^{\beta\alpha}(\mathbf{R})]_j}{E^{(\alpha)}(\mathbf{R}) - E^{(\beta)}(\mathbf{R})} \quad (14)$$

is a matrix determining position-dependent band parameters  $a(\mathbf{R})$ ,

$$\mathbf{p}_{nn'}^{\alpha\alpha'}(\mathbf{R}) = \sum_{\alpha'', \alpha'''} S^{+\alpha\alpha''}(\mathbf{R}) \mathbf{p}_{nn'}^{\alpha''\alpha'''} S^{\alpha'''\alpha'}(\mathbf{R}) \quad (15)$$

are position-dependent momentum operator matrix elements,  $\mathbf{p}_{nn'}^{(\alpha)}(\mathbf{R}) = \mathbf{p}_{nn'}^{\alpha\alpha}(\mathbf{R})$ . In the effective-mass approximation all position-dependent parameters in the bulk-like part of the Hamiltonian are proportional to the step-function  $\Theta(\mathbf{n}\mathbf{R})$ . The second term  $H_{nn'}^{S(\alpha)}(\hat{\mathbf{k}}, \mathbf{R})$ , which vanishes in the bulk material, is a short range part of the  $\mathbf{k}\mathbf{p}$ -Hamiltonian. It contains interface short range  $\delta$ -corrections, including terms proportional to  $n_i$ ,  $n_i n_j$ ,  $n_i \hat{k}_j$ ,  $n_i n_j \hat{k}_l$ ,  $\dots$ . In the effective mass approximation  $\delta^2(\mathbf{n}\mathbf{R}) \approx (1/a)\delta(\mathbf{n}\mathbf{R})$ ,  $\delta^3(\mathbf{n}\mathbf{R}) \approx (1/a^2)\delta(\mathbf{n}\mathbf{R})$ ,  $\dots$ , where  $a$  is a characteristic size of the interface region, and all parameters, which determine the short-range part of the Hamiltonian, are position-independent. In this approximation

$$H_{nn'}^{S(\alpha)}(\hat{\mathbf{k}}, \mathbf{R}) = \left[ \sum_i A_{nn'}^i n_i \delta(\mathbf{n}\mathbf{R}) + \sum_{i,j} B_{nn'}^{ij} n_i n_j \delta(\mathbf{n}\mathbf{R}) + \sum_{i,j} C_{nn'}^{ij} n_i \hat{k}_j \delta(\mathbf{n}\mathbf{R}) + \sum_{i,j,l} D_{nn'}^{ijl} \hat{k}_i \hat{k}_j n_l \delta(\mathbf{n}\mathbf{R}) + \sum_{i,j,l} K_{nn'}^{ijl} \hat{k}_i n_l \delta(\mathbf{n}\mathbf{R}) \hat{k}_j + \dots \right] + H.C.$$

All these terms can be introduced phenomenologically by the method of invariants, based only on the symmetry of the states under consideration (see Section III).



To take into account spin-orbit interaction it is necessary to add to the Hamiltonian (1) an operator  $H_{so}$ , which determines spin-orbit coupling. For heterosystems this operator includes three terms which mix states with different spin projections

$$H_{so} = \frac{\hbar}{4m_0^2c^2} ([\nabla U_1(\mathbf{x})\mathbf{p}] \cdot \sigma) + \frac{\hbar}{4m_0^2c^2} f(\mathbf{x}) ([\nabla (\Delta U(\mathbf{x}))\mathbf{p}] \cdot \sigma) + \frac{\hbar}{4m_0^2c^2} \Delta U(\mathbf{x}) ([\nabla f(\mathbf{x})\mathbf{p}] \cdot \sigma)$$

The first term in the right hand side of this expression is the usual operator of spin-orbit interaction in the bulk crystal with periodic potential  $U_1(\mathbf{x})$ . The second term determines the change of this operator across the interface. The third term is non-zero only in a narrow interface region and characterizes spin-dependent interface short range corrections.

Analysis shows that the spin-orbit coupling does not lead to a qualitative change of the effective Hamiltonian (12). The dependence  $E^{(\alpha)}(\mathbf{R})$  in (13) still determines the interface band offsets, but takes account of the position-dependent spin-orbit splitting. The matrix elements of momentum operator  $\mathbf{p}$  in (13)-(15) must be substituted by matrix elements of operator  $\pi$ , which in the case of a heterointerface system has the following form

$$\pi = \mathbf{p} + \frac{\hbar}{4m_0^2c^2} [\sigma \nabla U_1(\mathbf{x})] + \frac{\hbar}{4m_0^2c^2} f(\mathbf{x}) [\sigma \nabla (\Delta U(\mathbf{x}))].$$

All short range corrections, that arise due to the spin-orbit coupling, are relativistic and in the framework of the effective mass approximation can be included into the short range part of the Hamiltonian (12).

### III. **kp-HAMILTONIAN IN HETEROINTERFACE SYSTEM. METHOD OF INVARIANTS**

The effective Hamiltonian (12), containing real position-dependent band parameters  $a(\mathbf{R})$ , can be obtained by the method of invariants. To do that it is necessary to perform preliminary transformation to  $\mathbf{k}$ -representation. In this representation the matrix of the effective **kp**-Hamiltonian depends on the three variables  $\mathbf{k}$ ,  $\mathbf{k}'$  and  $\mathbf{n}$ , and includes Fourier transformants of the band parameters  $a(\mathbf{k} - \mathbf{k}')$  as "constants" of the method of invariants. This matrix must satisfy the invariance condition

$$\sum_{n'', n'''} D_{n'n''}^{(\alpha)}(g) H_{n''n'''}^{(\alpha)}(g^{-1}\mathbf{k}, g^{-1}\mathbf{k}'; g^{-1}\mathbf{n}) D_{n''n'}^{(\alpha)+}(g) = H_{nn'}^{(\alpha)}(\mathbf{k}, \mathbf{k}'; \mathbf{n}), \quad (16)$$

where  $D^{(\alpha)}(g)$  are the  $\Gamma_\alpha$  irreducible representation matrices of the crystal point-group  $F(g \in F)$ . The matrix of the Hamiltonian must be also Hermitian

$$H_{nn'}^{(\alpha)*}(\mathbf{k}, \mathbf{k}'; \mathbf{n}) = H_{n'n}^{(\alpha)}(\mathbf{k}', \mathbf{k}; \mathbf{n}) \quad (17)$$

and besides that it should satisfy the additional conditions of time-inversion invariance

$$H_{nn'}^{(\alpha*)}(-\mathbf{k}, -\mathbf{k}'; \mathbf{n}) = H_{nn'}^{(\alpha)*}(\mathbf{k}, \mathbf{k}'; \mathbf{n}). \quad (18)$$

Here  $|\alpha^*, n\rangle = T |\alpha, n\rangle$ , where  $T$  is the time-inversion operator.

Since the band parameters  $a(\mathbf{R})$  change only in the perpendicular to the interface direction, i.e. they are functions only of  $R_\perp = \mathbf{n}\mathbf{R}$ , their Fourier transformants are

$$a(\mathbf{k} - \mathbf{k}') = \frac{1}{V} \int a(\mathbf{R}) e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{R}} d\mathbf{R} = \frac{1}{V} \int a(R_\perp) e^{-i(k_\perp - k'_\perp)R_\perp} dR_\perp e^{-i(\mathbf{k}_\parallel - \mathbf{k}'_\parallel)\mathbf{R}_\parallel} d\mathbf{R}_\parallel = a(k_\perp - k'_\perp) \delta_{\mathbf{k}_\parallel \mathbf{k}'_\parallel},$$

where  $\mathbf{R}_\parallel = \mathbf{R} - \mathbf{n}R_\perp$ . These parameters are invariants under the symmetry transformation (16) and also satisfy the additional conditions (17) and (18).

The method of invariants allows one to obtain the matrix of the effective  $\mathbf{k}\mathbf{p}$ -Hamiltonian of the heterointerface system in any order of the perturbation theory in  $\mathbf{k}$  and  $\mathbf{n}$  with arbitrary "constants" (band parameters)  $a(\mathbf{k} - \mathbf{k}')$ .

We are mostly interested in  $A_3B_5$ -heterosystems (point-group  $T_d$ ). Table I. contains Hermitian combinations of  $\mathbf{k}$ ,  $\mathbf{k}'$  and  $\mathbf{n}$ , transforming according to irreducible representations of this group, up to the terms proportional  $kn^2$ .

TABLE I. Hermitian combinations of  $\mathbf{k}$ ,  $\mathbf{k}'$  and  $\mathbf{n}$ , transforming according to the irreducible representations of the point-group  $T_d$ .

Representation	Even under time inversion <sup>a</sup>	Odd under time inversion <sup>a</sup>
$\Gamma_{15}$	$i(\mathbf{k} - \mathbf{k}')$	$(\mathbf{k} + \mathbf{k}')$
$\Gamma_1$	$(\mathbf{k} \cdot \mathbf{k}')$	
$\Gamma_{12}$	$\begin{cases} 2k_z k'_z - k_x k'_x - k_y k'_y \\ \sqrt{3}(k_x k'_x - k_y k'_y) \end{cases}$	
$\Gamma_{15}$	$\{k_y k'_z\}, \{k_z k'_x\}, \{k_x k'_y\}$	
$\Gamma_{25}$		$i[\mathbf{k} \times \mathbf{k}']$
$\Gamma_{15}$	$\mathbf{n}$	
$\Gamma_1$	$(\mathbf{n} \cdot \mathbf{n}) = 1$	
$\Gamma_{12}$	$\begin{cases} 2n_z^2 - n_x^2 - n_y^2 \\ \sqrt{3}(n_x^2 - n_y^2) \end{cases}$	
$\Gamma_{15}$	$n_y n_z, n_z n_x, n_x n_y$	
$\Gamma_1$	$i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{n}$	$(\mathbf{k} + \mathbf{k}') \cdot \mathbf{n}$
$\Gamma_{12}$	$\begin{cases} i[2(k_z - k'_z)n_z - (k_x - k'_x)n_x \\ - (k_y - k'_y)n_y] \\ i\sqrt{3}[(k_x - k'_x)n_x - (k_y - k'_y)n_y] \end{cases}$	$\begin{cases} 2(k_z + k'_z)n_z - (k_x + k'_x)n_x \\ - (k_y + k'_y)n_y \\ \sqrt{3}[(k_x + k'_x)n_x - (k_y + k'_y)n_y] \end{cases}$
$\Gamma_{15}$	$\begin{cases} i\{(k_y - k'_y)n_z\} \\ i\{(k_z - k'_z)n_x\} \\ i\{(k_x - k'_x)n_y\} \end{cases}$	$\begin{cases} \{(k_y + k'_y)n_z\} \\ \{(k_z + k'_z)n_x\} \\ \{(k_x + k'_x)n_y\} \end{cases}$
$\Gamma_{25}$	$i[(\mathbf{k} - \mathbf{k}') \times \mathbf{n}]$	$[(\mathbf{k} + \mathbf{k}') \times \mathbf{n}]$
$\Gamma_{15}$	$i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{n}^2 = i(\mathbf{k} - \mathbf{k}')$	$(\mathbf{k} + \mathbf{k}') \cdot \mathbf{n}^2 = (\mathbf{k} + \mathbf{k}')$
$\Gamma_{15}$	$\begin{cases} i(k_x - k'_x)(2n_x^2 - n_y^2 - n_z^2) \\ i(k_y - k'_y)(2n_y^2 - n_z^2 - n_x^2) \\ i(k_z - k'_z)(2n_z^2 - n_x^2 - n_y^2) \end{cases}$	$\begin{cases} (k_x + k'_x)(2n_x^2 - n_y^2 - n_z^2) \\ (k_y + k'_y)(2n_y^2 - n_z^2 - n_x^2) \\ (k_z + k'_z)(2n_z^2 - n_x^2 - n_y^2) \end{cases}$
$\Gamma_{25}$	$\begin{cases} i(k_x - k'_x)(n_y^2 - n_z^2) \\ i(k_y - k'_y)(n_z^2 - n_x^2) \\ i(k_z - k'_z)(n_x^2 - n_y^2) \end{cases}$	$\begin{cases} (k_x + k'_x)(n_y^2 - n_z^2) \\ (k_y + k'_y)(n_z^2 - n_x^2) \\ (k_z + k'_z)(n_x^2 - n_y^2) \end{cases}$
$\Gamma_1$	$i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{N}$	$(\mathbf{k} + \mathbf{k}') \cdot \mathbf{N}$
$\Gamma_{12}$	$\begin{cases} i[2(k_z - k'_z)N_z - (k_x - k'_x)N_x \\ - (k_y - k'_y)N_y] \\ i\sqrt{3}[(k_x - k'_x)N_x - (k_y - k'_y)N_y] \end{cases}$	$\begin{cases} 2(k_z + k'_z)N_z - (k_x + k'_x)N_x \\ - (k_y + k'_y)N_y \\ \sqrt{3}[(k_x + k'_x)N_x - (k_y + k'_y)N_y] \end{cases}$
$\Gamma_{15}$	$\begin{cases} i\{(k_y - k'_y)N_z\} \\ i\{(k_z - k'_z)N_x\} \\ i\{(k_x - k'_x)N_y\} \end{cases}$	$\begin{cases} \{(k_y + k'_y)N_z\} \\ \{(k_z + k'_z)N_x\} \\ \{(k_x + k'_x)N_y\} \end{cases}$
$\Gamma_{25}$	$i[(\mathbf{k} - \mathbf{k}') \times \mathbf{N}]$	$[(\mathbf{k} + \mathbf{k}') \times \mathbf{N}]$

<sup>a</sup> $N_x = n_y n_z, N_y = n_z n_x, N_z = n_x n_y, \{A_i B_j\} = 1/2(A_i B_j + A_j B_i)$ .

Subsequent transformation to  $\mathbf{R}$ -representation is performed by the following rules:

$$a(\mathbf{k} - \mathbf{k}')(\mathbf{k} \pm \mathbf{k}') \longrightarrow \hat{\mathbf{k}}a(\mathbf{nR}) \pm a(\mathbf{nR})\hat{\mathbf{k}},$$

$$a(\mathbf{k} - \mathbf{k}')(k_i k'_j) \longrightarrow \hat{k}_i a(\mathbf{nR}) \hat{k}_j.$$

All the terms proportional to  $n_i$  and  $n_i n_j$  in  $\mathbf{R}$ -representation contain  $\delta$ -functions:

$$n_i \longrightarrow n_i \delta(\mathbf{nR}),$$

$$n_i n_j \longrightarrow n_i n_j \delta(\mathbf{nR}),$$

$$(k_i \pm k'_i) n_j \longrightarrow [\hat{k}_i \delta(\mathbf{nR}) \pm \delta(\mathbf{nR}) \hat{k}_i] n_j,$$

$$(k_i \pm k'_i) n_j n_l \longrightarrow [\hat{k}_i \delta(\mathbf{nR}) \pm \delta(\mathbf{nR}) \hat{k}_i] n_j n_l.$$

#### IV. EFFECTIVE HAMILTONIANS IN $A_3B_5$ -HETEROSYSTEMS

As it was mentioned above a single band Hamiltonian in a heterointerface system can be represented as a sum of bulk-like and short-range parts:

$$H^{(\alpha)}(\hat{\mathbf{k}}, \mathbf{R}) = H^{0(\alpha)}(\hat{\mathbf{k}}, \mathbf{R}) + H^{S(\alpha)}(\hat{\mathbf{k}}, \mathbf{R}).$$

The short range part  $H^{S(\alpha)}(\hat{\mathbf{k}}, \mathbf{R})$  contains terms proportional to  $n_i \delta(\mathbf{nR})$ ,  $n_i n_j \delta(\mathbf{nR})$ ,  $n_i \hat{k}_j \delta(\mathbf{nR})$ ,  $n_i \hat{k}_j \delta(\mathbf{nR}) \hat{k}_l$ ,  $\dots$ , which arise in the different orders of perturbation theory (11). These terms are interface short range corrections which change boundary conditions for smooth envelope functions in  $\mathbf{R}$ -representation. Analysis shows that in the short range part of the Hamiltonian it is sufficient to take into account only terms proportional to  $n$ ,  $n^2$ ,  $kn$ ,  $kn^2$ , since these corrections can provide proper form of subbands dispersion in quantum well, which is dictated by symmetry of the quantum well (e.g. point-group  $D_{2d}$  for a symmetric (001) quantum well). In this approximation the short range part of the Hamiltonian can be represented as a sum of four terms

$$H^{S(\alpha)}(\hat{\mathbf{k}}, \mathbf{R}) = H_n^{S(\alpha)}(\mathbf{R}) + H_{n^2}^{S(\alpha)}(\mathbf{R}) + H_{kn}^{S(\alpha)}(\hat{\mathbf{k}}, \mathbf{R}) + H_{kn^2}^{S(\alpha)}(\hat{\mathbf{k}}, \mathbf{R}).$$

In this Section the effective  $\mathbf{kp}$ -Hamiltonians of the  $\Gamma_1$ ,  $\Gamma_6$  and  $\Gamma_{15}$ ,  $\Gamma_8$  bands, and also  $\Gamma_8 \oplus \Gamma_7$  two-band Hamiltonian are presented. In the bulk-like part  $H^{0(\alpha)}(\hat{\mathbf{k}}, \mathbf{R})$  we considered  $E^{(\alpha)}(\mathbf{R}) = 0$  and took into account only terms up to quadratic-in- $\mathbf{k}$ . In the short range part we included only one term  $H_n^{S(\alpha)}(\mathbf{R})$ , proportional to the first order of  $\mathbf{n}$ , since it is the strongest short range correction, characterizing a uniform electric field localized in the interface region. The rest of the short range corrections are too cumbersome and therefore given in Appendix A.

It is necessary to note that the bulk-like part of the Hamiltonian  $H^{0(\alpha)}(\hat{\mathbf{k}}, \mathbf{R})$  includes position-dependent parameters, even though their explicit dependence on  $\mathbf{R}$  is omitted. Parameters that describe the short range part of the Hamiltonian  $H^{S(\alpha)}(\hat{\mathbf{k}}, \mathbf{R})$  are position-independent.

### A. $\Gamma_1$ band Hamiltonian

The  $\Gamma_1$  conduction band Hamiltonian is determined by one position-dependent parameter (inverse effective mass)  $a = m_0/m_e^*$ :

$$H^{0(\Gamma_1)}(\hat{\mathbf{k}}, \mathbf{R}) = \frac{\hbar^2}{2m_0} (\hat{\mathbf{k}} a \hat{\mathbf{k}}).$$

Here  $(\hat{\mathbf{k}} a \hat{\mathbf{k}}) = \hat{k}_x a \hat{k}_x + \hat{k}_y a \hat{k}_y + \hat{k}_z a \hat{k}_z$ ,  $a = 1 + \frac{2}{m_0} \sum_q \frac{|\langle \Gamma_{15}; q | \mathbf{p} | \Gamma_1 \rangle|^2}{E_{\Gamma_1} - E_q^{\Gamma_{15}}}$ .

The short range terms, proportional to the first order of  $\mathbf{n}$ , in the  $\Gamma_1$  band Hamiltonian do not exist ( $H_n^{S(\Gamma_1)}(\mathbf{R}) = 0$ ).

### B. $\Gamma_6$ band Hamiltonian

The  $\Gamma_6$  conduction band Hamiltonian is determined by two position-dependent parameters  $\alpha_1$  and  $\alpha_2$

$$H^{0(\Gamma_6)}(\hat{\mathbf{k}}, \mathbf{R}) = \frac{\hbar^2}{2m_0} \left[ (\hat{\mathbf{k}} \alpha_1 \hat{\mathbf{k}}) I + i \left( [\hat{\mathbf{k}} \alpha_2 \hat{\mathbf{k}}] \cdot \boldsymbol{\sigma} \right) \right].$$

Here  $I$  is a unit matrix  $2 \times 2$ ,  $\sigma_i$  are Pauli matrices,  $[\hat{\mathbf{k}} a \hat{\mathbf{k}}]_i = \hat{k}_{i+1} a \hat{k}_{i+2} - \hat{k}_{i+2} a \hat{k}_{i+1}$ .

The parameter  $\alpha_1 = m_0/m_e^*$  determines the electron inverse effective mass in the  $\Gamma_6$  band and is equal to the parameter  $a$  of the  $\Gamma_1$  band, when we neglect spin-orbit coupling. The parameter  $\alpha_2$  determines an additional relativistic term, which arises when the presence of heterointerface is taken into account. It vanishes in the bulk material due to commutativity of  $\alpha_2$  and operator  $\hat{\mathbf{k}}$ . This term describes electron effective spin-orbit coupling at the heterointerface, which is calculated by means of envelope functions (interface effective spin-orbit interaction). Indeed, using the commutation relation  $\alpha_2(\mathbf{R}) \hat{\mathbf{k}} - \hat{\mathbf{k}} \alpha_2(\mathbf{R}) = i \partial \alpha_2(\mathbf{R}) / \partial \mathbf{R}$  and taking into account the fact that in the effective mass approximation  $\partial \alpha_2(\mathbf{R}) / \partial \mathbf{R} \approx \Delta \alpha_2 \mathbf{n} \delta(\mathbf{nR})$ , this term can be represented in the form  $\Delta \alpha_2 \left( [\mathbf{n} \times \hat{\mathbf{k}}] \cdot \boldsymbol{\sigma} \right) \delta(\mathbf{nR})$ . It is easy to see that it is analogous to the operator of spin-orbit interaction, in which the factor proportional to  $\Delta \alpha_2 \mathbf{n} \delta(\mathbf{nR})$  acts as an effective electric field localized in the interface region and  $\hat{\mathbf{k}}$  is the momentum operator in the effective mass approximation.

The parameter  $\alpha_2$  can be approximately determined if we take into account  $\mathbf{k}\mathbf{p}$ -interaction of the  $\Gamma_6(\Gamma_1^c)$  conduction band only with the  $\Gamma_8 \oplus \Gamma_7(\Gamma_{15}^v)$  valence band. In

this approximation it is proportional to the spin-orbit splitting of the  $\Gamma_{15}^v$  band and to the square of the matrix element  $\langle \Gamma_{15}^v \| \mathbf{p} \| \Gamma_1^c \rangle$ , which determines the electron effective mass in the  $\Gamma_6(\Gamma_1^c)$  band. Thus it can be approximately represented as

$$\alpha_2 = [\Delta_{so}/(3E_g + 2\Delta_{so})] (1 - m_0/m_e),$$

where  $E_g = E_c^{\Gamma_6} - E_v^{\Gamma_8}$ ,  $\Delta_{so} = E_v^{\Gamma_8} - E_v^{\Gamma_7}$  is the spin-orbit splitting of the  $\Gamma_{15}^v$  band.

The short range part, proportional to the first order of  $\mathbf{n}$ , in the  $\Gamma_6$  band Hamiltonian does not exist ( $H_n^{S(\Gamma_6)}(\mathbf{R}) = 0$ ).

### C. $\Gamma_{15}$ band Hamiltonian

The bulk-like part of the  $\Gamma_{15}$  band hole Hamiltonian, containing four quadratic-in- $\mathbf{k}$  terms and one linear-in- $\mathbf{k}$  term, can be written in the form

$$H^{0(\Gamma_{15})}(\hat{\mathbf{k}}, \mathbf{R}) = \frac{\hbar^2}{2m_0} \left[ (\hat{\mathbf{k}}b_1\hat{\mathbf{k}}) I - 6 \sum_i \left[ \hat{k}_i b_2 \hat{k}_i - \frac{1}{3} (\hat{\mathbf{k}}b_2\hat{\mathbf{k}}) \right] J_i^2 - \right. \\ \left. 12 \sum_i \left\{ \hat{k}_i b_3 \hat{k}_{i+1} \right\} \{J_i J_{i+1}\} + i3 \left( [\hat{\mathbf{k}}b_4\hat{\mathbf{k}}] \cdot \mathbf{J} \right) + \frac{i}{a_0} 2\sqrt{3} \sum_i [\hat{k}_i d] \{J_{i+1} J_{i+2}\} \right],$$

where  $I$  is a unit matrix  $3 \times 3$ ,  $J_i$  are matrices of the angular momentum  $J = 1$ ,  $\{J_i J_j\} = \frac{1}{2} (J_i J_j + J_j J_i)$ ,  $\{\hat{k}_i a \hat{k}_j\} = \frac{1}{2} (\hat{k}_i a \hat{k}_j + \hat{k}_j a \hat{k}_i)$ ,  $[\hat{k}_i d] = \hat{k}_i d - d \hat{k}_i$ ,  $a_0$  is the lattice constant, which was introduced for convenience.

Band parameters  $b_l$  can be expressed by position-dependent parameters  $\rho_l$ , which describe  $\mathbf{k}\mathbf{p}$ -interaction of the  $\Gamma_{15}$  valence band with the  $\Gamma_1$ ,  $\Gamma_{12}$ ,  $\Gamma_{15}$  and  $\Gamma_{25}$  bands:

$$b_1 = -1 + 2\rho_1 + 4\rho_2 + 4\rho_3 + 4\rho_4,$$

$$b_2 = \rho_1 - \rho_2 - \rho_3 + 2\rho_4,$$

$$b_3 = \rho_1 - \rho_2 + \rho_3 - \rho_4,$$

$$b_4 = \rho_1 + \rho_2 - \rho_3 - \rho_4.$$

Here

$$\rho_1 = \frac{1}{3m_0} \sum_q \frac{|\langle \Gamma_{15} \| \mathbf{p} \| \Gamma_1; q \rangle|^2}{E_q^{\Gamma_1} - E^{\Gamma_{15}}},$$

$$\begin{aligned}\rho_2 &= \frac{1}{6m_0} \sum_q \frac{|\langle \Gamma_{15} \| \mathbf{p} \| \Gamma_{25}; q \rangle|^2}{E_q^{\Gamma_{25}} - E^{\Gamma_{15}}}, \\ \rho_3 &= \frac{1}{6m_0} \sum_q \frac{|\langle \Gamma_{15} \| \mathbf{p} \| \Gamma_{15}; q \rangle|^2}{E_q^{\Gamma_{15}} - E^{\Gamma_{15}}}, \\ \rho_4 &= \frac{1}{6m_0} \sum_q \frac{|\langle \Gamma_{15} \| \mathbf{p} \| \Gamma_{12}; q \rangle|^2}{E_q^{\Gamma_{12}} - E^{\Gamma_{15}}}.\end{aligned}$$

The position-dependent parameters  $b_1$ ,  $b_2$  and  $b_3$  are analogous to the  $\Gamma_{15}$  band parameters of the bulk material. The parameter  $b_4$  arises due to the presence of the heterointerface and similarly to the parameter  $\alpha_2$  of the  $\Gamma_6$  band describes interface effective spin-orbit interaction. In this case hole in the  $\Gamma_{15}$  band should be attributed an effective spin  $J = 1$ . If  $\mathbf{k}\mathbf{p}$ -interaction of the  $\Gamma_{15}$  valence band with all the  $\Gamma_{25}$  bands is neglected ( $\rho_2 = 0$ ) the parameter  $b_4$  can be expressed by all other parameters  $b_1$ ,  $b_2$  and  $b_3$ . In this approximation  $b_4 = (1/3)(-1 - b_1 + 2b_2 + 3b_3)$ .

The additional linear-in- $\mathbf{k}$  term, which is proportional to a position-dependent parameter  $d$ , appears in the  $\Gamma_{15}$  band  $\mathbf{k}\mathbf{p}$ -Hamiltonian only when the presence of interface is taken into account and arises due to variation of the Bloch functions across the interface. Indeed, the diagonal matrix elements of the momentum operator  $\mathbf{p}_{nn'}^{\Gamma_{15}\Gamma_{15}} = \mathbf{p}_{nn'}^{(\Gamma_{15})}$  are equal to zero since the operator  $\mathbf{p}$  is odd under time inversion. However, this does not take place when the position-dependent pseudo-coordinate basis is used, since in this case, according to (15), the diagonal position-dependent matrix elements of the momentum operator also include off-diagonal matrix elements of the operator  $\mathbf{p}$ , which are non-zero in general

$$\mathbf{p}_{nn'}^{(\Gamma_{15})}(\mathbf{R}) = \sum_{\Gamma'_{15}\Gamma''_{15}} S^{+\Gamma_{15}\Gamma'_{15}}(\mathbf{R}) \mathbf{p}_{nn'}^{\Gamma'_{15}\Gamma''_{15}} S^{\Gamma''_{15}\Gamma_{15}}(\mathbf{R}).$$

The short range part of the  $\Gamma_{15}$  band Hamiltonian, which is proportional to the first order of  $\mathbf{n}$ , is determined by one position-independent parameter  $r$  and has the form

$$H_n^{S(\Gamma_{15})}(\mathbf{R}) = \frac{\hbar^2}{2m_0 a_0} 2\sqrt{3}r \sum_i n_i \{J_{i+1} J_{i+2}\} \delta(\mathbf{n}\mathbf{R}).$$

This short range correction coincides with the correction, introduced in Ref. [14]. for the case of (001) interface, and generalizes it for arbitrary interface orientation.

#### D. $\Gamma_8$ band Hamiltonian

The bulk-like part of the  $\Gamma_8$  band hole Hamiltonian along with the usual quadratic-in- $\mathbf{k}$  terms, determined by position-dependent Luttinger parameters  $\gamma_1$ ,  $\gamma_2$  and  $\gamma_3$ , is also characterized by two additional quadratic-in- $\mathbf{k}$  terms, determined by parameters  $\gamma_4$  and  $\gamma_5$ , and two linear-in- $\mathbf{k}$  terms, described by parameters  $\beta_1$  and  $\beta_2$

$$H^{0(\Gamma_8)}(\hat{\mathbf{k}}, \mathbf{R}) = \frac{\hbar^2}{2m_0} \left[ (\hat{\mathbf{k}}\gamma_1\hat{\mathbf{k}}) I - 2 \sum_i \left[ \hat{k}_i\gamma_2\hat{k}_i - \frac{1}{3} (\hat{\mathbf{k}}\gamma_2\hat{\mathbf{k}}) \right] J_i^2 - 4 \sum_i \left\{ \hat{k}_i\gamma_3\hat{k}_{i+1} \right\} \{J_i J_{i+1}\} + i2 \left( [\hat{\mathbf{k}}\gamma_4\hat{\mathbf{k}}] \cdot \mathbf{J} \right) + i8 \sum_i [\hat{\mathbf{k}}\gamma_5\hat{\mathbf{k}}]_i J_i^3 + \frac{i}{a_0} \frac{2}{\sqrt{3}} \sum_i [\hat{k}_i\beta_1] \{J_{i+1}J_{i+2}\} + \frac{1}{a_0} \frac{4}{\sqrt{3}} \sum_i \left\{ \hat{k}_i\beta_2 \right\} \left\{ J_i (J_{i+1}^2 - J_{i+2}^2) \right\} \right],$$

where  $I$  is a unit matrix  $4 \times 4$ ,  $J_i$  are matrix of the angular momentum  $J = 3/2$ ,  $\{\hat{k}_i a\} = \frac{1}{2} (\hat{k}_i a + a \hat{k}_i)$ .

Neglecting spin-orbit interaction, the  $\Gamma_8$  band parameters can be determined by the  $\Gamma_{15}$  valence band parameters  $b_l$ :  $\gamma_1 = b_1$ ,  $\gamma_2 = b_2$ ,  $\gamma_3 = b_3$ ,  $\gamma_4 = b_4$ . The additional parameters  $\gamma_4$  and  $\gamma_5$ , which describe quadratic-in- $\mathbf{k}$  terms, arise due to interface effective spin-orbit interaction, calculated by means of envelope functions (the hole effective spin  $J = 3/2$ ). The parameter  $\gamma_4$  is non-relativistic and can be determined approximately by the Luttinger parameters if  $\mathbf{k}\mathbf{p}$ -interaction of the  $\Gamma_{15}^v$  band with all the  $\Gamma_{25}$  bands is neglected (i.e.  $\rho_2 = 0$ ). In this case  $\gamma_4 = (1/3)(-1 - \gamma_1 + 2\gamma_2 + 3\gamma_3)$ . The first four terms of the  $\Gamma_8$  valence band  $\mathbf{k}\mathbf{p}$ -Hamiltonian, which are proportional to the parameters  $\gamma_1$ ,  $\gamma_2$ ,  $\gamma_3$  and  $\gamma_4$ , coincide with  $\mathbf{k}\mathbf{p}$ -Hamiltonian obtained by Foreman in Ref. [10]. The parameter  $\gamma_5$  is non-zero only if spin-orbit splitting of the intermediate states in the  $\mathbf{k}\mathbf{p}$ -perturbation theory is taken into account. This parameter can be approximately determined, by taking into account  $\mathbf{k}\mathbf{p}$ -interaction of the  $\Gamma_8(\Gamma_{15}^v)$  valence band only with the nearest  $\Gamma_7 \oplus \Gamma_8(\Gamma_{15}^c)$  conduction band. Then it is  $\gamma_5 = (1/18)(1 + \gamma_1 - 2\gamma_2) [\Delta'_{so}/(E'_g + \Delta'_{so})]$ , where  $E'_g = E_c^{\Gamma_7} - E_v^{\Gamma_8}$ ,  $\Delta'_{so} = E_c^{\Gamma_8} - E_c^{\Gamma_7}$  is the spin-orbit splitting of the  $\Gamma_{15}^c$  conduction band.

The hole  $\Gamma_8$  band Hamiltonian contains two linear-in- $\mathbf{k}$  terms, determined by the parameters  $\beta_1$  and  $\beta_2$ . The parameter  $\beta_1$ , which arises due to variation of the Bloch functions across the interface, is non-relativistic and is originated from the corresponding parameter  $d$  of the  $\Gamma_{15}$  band ( $\beta_1 = d$  if spin-orbit coupling is neglected). The parameter  $\beta_2$  is relativistic and analogous to the corresponding parameter of the  $\Gamma_8$  band in the bulk material, that arises due to the absence of the inversion symmetry in  $A_3B_5$ -semiconductors.

The short range part of the  $\Gamma_8$  band Hamiltonian, which is proportional to the first order of  $\mathbf{n}$ , is determined by one parameter  $\nu$ , which is originated from the corresponding parameter  $r$  of the  $\Gamma_{15}$  band (when the spin-orbit coupling is neglected  $\nu = r$ ) and has the form



$$H_n^{S(\Gamma_8)}(\mathbf{R}) = \frac{\hbar^2}{2m_0 a_0} \frac{2}{\sqrt{3}} \nu \sum_i n_i \{J_{i+1} J_{i+2}\} \delta(\mathbf{nR}).$$

### E. Two-band $\Gamma_8 \oplus \Gamma_7$ Hamiltonian

The  $\Gamma_8 \oplus \Gamma_7$  two-band hole Hamiltonian can be represented in the following matrix form:

$$H^{(\Gamma_8 \oplus \Gamma_7)}(\hat{\mathbf{k}}, \mathbf{R}) = \begin{bmatrix} H^{(\Gamma_8)}(\hat{\mathbf{k}}, \mathbf{R}) & H^{(\Gamma_8 \Gamma_7)}(\hat{\mathbf{k}}, \mathbf{R}) \\ H^{(\Gamma_8 \Gamma_7)^+}(\hat{\mathbf{k}}, \mathbf{R}) & H^{(\Gamma_7)}(\hat{\mathbf{k}}, \mathbf{R}) \end{bmatrix}.$$

Parameters that determine this Hamiltonian can be approximately related to corresponding parameters of the  $\Gamma_8(\Gamma_{15}^v)$  band Hamiltonian if we neglect spin-orbit mixing. In this case  $H^{(\Gamma_8)}(\hat{\mathbf{k}}, \mathbf{R})$  coincides with the  $\Gamma_8$  band Hamiltonian (see Section IV.D), in which  $\gamma_5 = \beta_2 = 0$ . Note that the  $\Gamma_7$  band Hamiltonian also includes a term which describe interface effective spin-orbit interaction. However in contrast to the  $\Gamma_6(\Gamma_1^c)$  band Hamiltonian this term is non-relativistic and proportional to the parameter  $\gamma_4$ . Also in this approximation the  $H^{0(\Gamma_8 \Gamma_7)}(\hat{\mathbf{k}}, \mathbf{R})$  block contains one linear-in- $\mathbf{k}$  term proportional to the parameter  $\beta_1$

$$\begin{aligned} H^{0(\Gamma_7)}(\hat{\mathbf{k}}, \mathbf{R}) &= \Delta_{so} I + \frac{\hbar^2}{2m_0} \left[ (\hat{\mathbf{k}} \gamma_1 \hat{\mathbf{k}}) I + i2 \left( [\hat{\mathbf{k}} \gamma_4 \hat{\mathbf{k}}] \cdot \sigma \right) \right], \\ H^{0(\Gamma_8 \Gamma_7)}(\hat{\mathbf{k}}, \mathbf{R}) &= \frac{\hbar^2}{2m_0} \left[ -\sqrt{2} \left[ (2\hat{k}_z \gamma_2 \hat{k}_z - \hat{k}_x \gamma_2 \hat{k}_x - \hat{k}_y \gamma_2 \hat{k}_y) I_1^{\Gamma_{12}} - \right. \right. \\ &\quad \left. \left. \sqrt{3} (\hat{k}_x \gamma_2 \hat{k}_x - \hat{k}_y \gamma_2 \hat{k}_y) I_2^{\Gamma_{12}} \right] - \sqrt{6} \sum_i \{ \hat{k}_{i+1} \gamma_3 \hat{k}_{i+2} \} I_i^{\Gamma_{15}} + \right. \\ &\quad \left. i \frac{1}{\sqrt{2}} \sum_i [\hat{k}_{i+1} \gamma_4 \hat{k}_{i+2}] I_i^{\Gamma_{25}} + \frac{i}{a_0} \frac{1}{\sqrt{2}} \sum_i [\hat{k}_i \beta_1] I_i^{\Gamma_{15}} \right], \end{aligned}$$

where  $I$  is a unit matrix  $2 \times 2$ ,  $\Delta_{so} = E_v^{\Gamma_8} - E_v^{\Gamma_7}$ , matrices  $I_i^{\Gamma_\alpha}$  are given in Appendix B.

The short range part of this Hamiltonian, which is proportional to the first order of  $\mathbf{n}$ , can be described by the corresponding parameters of the  $\Gamma_8$  band

$$H_n^{S(\Gamma_7)}(\mathbf{R}) = 0,$$

$$H_n^{S(\Gamma_8 \Gamma_7)}(\mathbf{R}) = \frac{\hbar^2}{2m_0 a_0} \frac{1}{\sqrt{2}} \nu \sum_i n_i I_i^{\Gamma_{15}} \delta(\mathbf{nR}).$$

### V. BOUNDARY CONDITIONS

The boundary conditions for envelope functions can be obtained by integrating the effective-mass equation

$$\sum_{n'} H_{nn'}^{(\alpha)}(\hat{\mathbf{k}}, \mathbf{R}) \psi_{n'}^{(\alpha)}(\mathbf{R}) = E^{(\alpha)} \psi_n^{(\alpha)}(\mathbf{R}),$$

along the normal  $\mathbf{n}$  across the interface. Taking into account in the effective-mass Hamiltonian  $H^{(\alpha)}(\hat{\mathbf{k}}, \mathbf{R})$  only bulk-like part  $H^{0(\alpha)}(\hat{\mathbf{k}}, \mathbf{R})$  and main short range term  $H_n^{(\alpha)}(\hat{\mathbf{k}}, \mathbf{R})$ , proportional to the first order of  $\mathbf{n}$ , we obtain the following boundary conditions, that depend on the interface orientation

$$\psi|_{\mathbf{nR}=+0} = \psi|_{\mathbf{nR}=-0},$$

$$(\hat{A}_{\mathbf{nR}}\psi)|_{\mathbf{nR}=+0} - (\hat{A}_{\mathbf{nR}}\psi)|_{\mathbf{nR}=-0} = B_{\mathbf{nR}}\psi|_{\mathbf{nR}=0},$$

here matrix operator  $\hat{A}_{\mathbf{nR}}$  is determined by the bulk-like part  $H^{0(\alpha)}(\hat{\mathbf{k}}, \mathbf{R})$  of the Hamiltonian, and matrix  $B_{\mathbf{nR}}$  by its short range part  $H_n^{S(\alpha)}(\hat{\mathbf{k}}, \mathbf{R})$ .

The matrices  $\hat{A}_{\mathbf{nR}}$  and  $B_{\mathbf{nR}}$ , that determine boundary conditions for all the bands discussed in this paper, are given below for the case of (001) interface, when  $n_x = n_y = 0$ ,  $n_z = 1$  ( $\mathbf{nR} = z$ ).

#### A. $\Gamma_1$ band boundary conditions

$$\hat{A}_z^{(\Gamma_1)} = \frac{\hbar^2}{2m_0} (a\hat{k}_z),$$

$$B_z^{(\Gamma_1)} = 0.$$

#### B. $\Gamma_6$ band boundary conditions

$$\hat{A}_z^{(\Gamma_6)} = \frac{\hbar^2}{2m_0} \left[ (\alpha_1 \hat{k}_z) I + i\alpha_2 (-\sigma_x \hat{k}_y + \sigma_y \hat{k}_x) \right],$$

$$B_z^{(\Gamma_6)} = 0.$$

#### C. $\Gamma_{15}$ band boundary conditions

$$\hat{A}_z^{(\Gamma_{15})} = \frac{\hbar^2}{2m_0} \left[ (b_1 \hat{k}_z) I - 2b_2 (2J_z^2 - J_x^2 - J_y^2) \hat{k}_z - \right. \\ \left. 6b_3 (\{J_y J_z\} \hat{k}_y + \{J_z J_x\} \hat{k}_x) + i3b_4 (-J_x \hat{k}_y + J_y \hat{k}_x) + \frac{i}{a_0} 2\sqrt{3}d \{J_x J_y\} \right],$$

$$B_z^{(\Gamma_{15})} = -i \frac{\hbar^2}{2m_0 a_0} 2\sqrt{3}r \{J_x J_y\}.$$

#### D. $\Gamma_8$ band boundary conditions

$$\hat{A}_z^{(\Gamma_8)} = \frac{\hbar^2}{2m_0} \left[ (\gamma_1 \hat{k}_z) I - \frac{2}{3}\gamma_2 (2J_z^2 - J_x^2 - J_y^2) \hat{k}_z - \right. \\ \left. 2\gamma_3 (\{J_y J_z\} \hat{k}_y + \{J_z J_x\} \hat{k}_x) + i2\gamma_4 (-J_x \hat{k}_y + J_y \hat{k}_x) + i8\gamma_5 (-J_x^3 \hat{k}_y + J_y^3 \hat{k}_x) + \right. \\ \left. \frac{i}{a_0} \frac{2}{\sqrt{3}}\beta_1 \{J_x J_y\} + \frac{1}{a_0} \frac{4}{\sqrt{3}}\beta_2 \{J_z (J_x^2 - J_y^2)\} \right],$$

$$B_z^{(\Gamma_8)} = -i \frac{\hbar^2}{2m_0 a_0} \frac{2}{\sqrt{3}}\nu \{J_x J_y\}.$$

#### E. $\Gamma_8 \oplus \Gamma_7$ band boundary conditions

$$\hat{A}_z^{(\Gamma_8 \oplus \Gamma_7)} = \begin{bmatrix} \hat{A}_z^{(\Gamma_8)} & \hat{A}_z^{(\Gamma_8 \Gamma_7)} \\ \hat{A}_z^{(\Gamma_8 \Gamma_7)+} & \hat{A}_z^{(\Gamma_7)} \end{bmatrix},$$

$$B_z^{(\Gamma_8 \oplus \Gamma_7)} = \begin{bmatrix} B_z^{(\Gamma_8)} & B_z^{(\Gamma_8 \Gamma_7)} \\ B_z^{(\Gamma_8 \Gamma_7)+} & B_z^{(\Gamma_7)} \end{bmatrix},$$

where  $\hat{A}_z^{(\Gamma_8)}$  and  $B_z^{(\Gamma_8)}$  coincide with corresponding matrices of the  $\Gamma_8$  band (see Section V. D.), in which  $\gamma_5 = 0$  and  $\beta_2 = 0$ .

$$\hat{A}_z^{(\Gamma_7)} = \frac{\hbar^2}{2m_0} \left[ (\gamma_1 \hat{k}_z) I + i2\gamma_4 (-\sigma_x \hat{k}_y + \sigma_y \hat{k}_x) \right],$$

$$\hat{A}_z^{(\Gamma_8 \Gamma_7)} = \frac{\hbar^2}{2m_0} \left[ -2\sqrt{2}\gamma_2 I_1^{\Gamma_{12}} \hat{k}_z - \sqrt{6}\gamma_3 (I_x^{\Gamma_{15}} \hat{k}_y + I_y^{\Gamma_{15}} \hat{k}_x) + \right. \\ \left. i\frac{1}{\sqrt{2}}\gamma_4 (-I_x^{\Gamma_{25}} \hat{k}_y + I_y^{\Gamma_{25}} \hat{k}_x) + \frac{i}{a_0} \frac{1}{\sqrt{2}}\beta_1 I_z^{\Gamma_{15}} \right],$$

$$B_z^{(\Gamma_7)} = 0,$$

$$B_z^{(\Gamma_8\Gamma_7)} = -i\frac{\hbar^2}{2m_0a_0}\frac{1}{\sqrt{2}}\nu I_z^{\Gamma_{15}}.$$

The  $\mathbf{k}$ -dependent short range terms, which were not included into the boundary conditions, along with  $\delta$ -functions contain also their derivatives, which modify the boundary conditions. However, influence of the omitted corrections is small and therefore when considering systems with heterointerface (e.g. quantum well) it is more convenient to take these corrections into account by the perturbation theory in the framework of the envelope function approximation.

## V. SUMMARY

In this paper using a position-dependent pseudo-coordinate basis the effective mass equation for electrons and holes in heterosystems for arbitrary interface orientation is obtained. Using this basis one can exclude off-diagonal matrix elements of the interface scattering potential and in the explicit form introduce into the theory position-dependent parameters, that describe bulk material (electron energy at  $\mathbf{k} = 0$  and band parameters) and can be taken from experiment. This approach is close to the theories developed by Karavaev and Tikhodeev [3] and Foreman [8], [10].

To obtain the effective  $\mathbf{kp}$ -Hamiltonians with position-dependent parameters in  $A_3B_5$ -heterointerface systems a modified method of invariants is suggested. Since the presence of interface disturbs translational symmetry of the crystal and leads to scattering of the particles, changing their wave vector from  $\mathbf{k}$  to  $\mathbf{k}'$ , the effective Hamiltonian of the heterosystem, in contrast to the bulk material, should be considered dependent on these two variables. Besides that the effective  $\mathbf{kp}$ -Hamiltonian has to depend on the interface orientation, and therefore it should be described by one more independent variable  $\mathbf{n}$  (the normal to the interface). Using this approach we obtained for arbitrary interface orientation the effective  $\mathbf{kp}$ -Hamiltonians with position-dependent band parameters for the  $\Gamma_1$  and  $\Gamma_6$  conduction bands,  $\Gamma_{15}$  and  $\Gamma_8$  valence bands, and also  $\Gamma_8 \oplus \Gamma_7$  two-band effective  $\mathbf{kp}$ -Hamiltonian.

In the framework of this approach the effective  $\mathbf{kp}$ -Hamiltonian with position-dependent parameters can be represented as a sum of two parts: bulk-like part  $H^{0(\alpha)}$  and short range part  $H^{S(\alpha)}$ . The bulk-like part, along with the usual terms, that are present in the Hamiltonian of a homogenous material, also includes additional quadratic-in- $\mathbf{k}$  terms. They arise due to non-commutativity of the momentum operator and band parameters and vanish in the bulk material. Analysis shows that these

terms describe effective spin-orbit coupling at the interface and lead to spin-dependent effects of electron and hole interface scattering.

Besides that the bulk-like part of the **kp**-Hamiltonian  $H^{0(\alpha)}$  can include non-relativistic linear-in-**k** term, that appears due to variation of the Bloch functions across the interface. The short-range part  $H^{S(\alpha)}$  includes terms proportional to  $n$ ,  $n^2$ ,  $nk$ ,  $nk^2$ ,  $\dots$ . The terms proportional to the first order of **n**, which characterize the uniform electric field localized in the interface region, are the most important. In particular, in the  $\Gamma_8$  band these corrections lead to a well known effect of heavy-light holes mixing at the interface. Analysis shows that  $kn$  and  $kn^2$  type terms are responsible for linear-in-**k** Rashba-like terms in the electron and hole subbands dispersion in quantum wells. Influence of these terms on the effect can exceed the contribution of the cubic-in-**k** terms, which exist in the bulk Hamiltonian of the  $A_3B_5$ -semiconductors due to absence of the inversion symmetry.

The effective Hamiltonians derived in this paper allow one to obtain the correct boundary conditions for electron and hole envelope functions for arbitrary interface orientation. The additional terms, which were introduced into the Hamiltonians in this paper, modify usually used boundary conditions. However, some short range corrections (for example  $n^2$ ,  $nk$ ,  $nk^2$  type terms) are small and can be easily taken into account by the perturbation theory in the framework of the envelope function approximation.

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## APPENDIX A: HIGH ORDERS SHORT RANGE PARTS OF THE HAMILTONIANS

### A1. $\Gamma_1$ band Hamiltonian

$$H_{n^2}^{S(\Gamma_1)}(\mathbf{R}) = \frac{\hbar^2}{2m_0a_0}g(\mathbf{n} \cdot \mathbf{n})\delta(\mathbf{nR}),$$

$$H_{kn}^{S(\Gamma_1)}(\hat{\mathbf{k}}, \mathbf{R}) = i\frac{\hbar^2}{2m_0}l\left(\left[\hat{\mathbf{k}}\delta\right] \cdot \mathbf{n}\right),$$

$$H_{kn^2}^{S(\Gamma_1)}(\hat{\mathbf{k}}, \mathbf{R}) = i\frac{\hbar^2}{2m_0}q\left(\left[\hat{\mathbf{k}}\delta\right] \cdot \mathbf{N}\right).$$

Here  $\left[\hat{\mathbf{k}}\delta\right] = \hat{\mathbf{k}}\delta(\mathbf{nR}) - \delta(\mathbf{nR})\hat{\mathbf{k}}$ .

### A2. $\Gamma_6$ band Hamiltonian

$$\begin{aligned}
H_{n^2}^{S(\Gamma_6)}(\mathbf{R}) &= \frac{\hbar^2}{2m_0a_0} \eta(\mathbf{n} \cdot \mathbf{n}) I \delta(\mathbf{nR}), \\
H_{kn}^{S(\Gamma_6)}(\hat{\mathbf{k}}, \mathbf{R}) &= \frac{\hbar^2}{2m_0} \left[ i\lambda_1 \left( [\hat{\mathbf{k}}\delta] \cdot \mathbf{n} \right) I + \lambda_2 \left( [\{\hat{\mathbf{k}}\delta\} \times \mathbf{n}] \cdot \sigma \right) \right], \\
H_{kn^2}^{S(\Gamma_6)}(\hat{\mathbf{k}}, \mathbf{R}) &= \frac{\hbar^2}{2m_0} \left[ i\mu_1 \left( [\hat{\mathbf{k}}\delta] \cdot \mathbf{N} \right) I + \mu_2 \sum_i \left\{ \hat{k}_i \delta \right\} (n_{i+1}^2 - n_{i+2}^2) \sigma_i + \right. \\
&\quad \left. \mu_3 \left( [\{\hat{\mathbf{k}}\delta\} \times \mathbf{N}] \cdot \sigma \right) \right].
\end{aligned}$$

Here  $\{\hat{\mathbf{k}}\delta\} = \frac{1}{2} [\hat{\mathbf{k}}\delta(\mathbf{nR}) + \delta(\mathbf{nR})\hat{\mathbf{k}}]$ ,  $I$  is a unit matrix  $2 \times 2$ ,  $\sigma_i$  are Pauli matrices. If we neglect spin-orbit mixing  $\eta = g$ ,  $\lambda_1 = l$ ,  $\mu_1 = q$  and  $\lambda_2 = \mu_2 = \mu_3 = 0$ .

### A3. $\Gamma_{15}$ band Hamiltonian

$$\begin{aligned}
H_{n^2}^{S(\Gamma_{15})}(\mathbf{R}) &= \frac{\hbar^2}{2m_0a_0} \left[ s_1(\mathbf{n} \cdot \mathbf{n}) I \delta(\mathbf{nR}) + 6s_2 \sum_i (n_i^2 - \frac{1}{3}) J_i^2 \delta(\mathbf{nR}) + \right. \\
&\quad \left. 12s_3 \sum_i N_i \{J_{i+1} J_{i+2}\} \delta(\mathbf{nR}) \right], \\
H_{kn}^{S(\Gamma_{15})}(\hat{\mathbf{k}}, \mathbf{R}) &= \frac{\hbar^2}{2m_0} \left[ it_1 \left( [\hat{\mathbf{k}}\delta] \cdot \mathbf{n} \right) I + i6t_2 \sum_i \left( [\hat{k}_i \delta] n_i - \frac{1}{3} ([\hat{\mathbf{k}}\delta] \cdot \mathbf{n}) \right) J_i^2 + \right. \\
&\quad \left. i12t_3 \sum_i \left\{ [\hat{k}_i \delta] n_{i+1} \right\} \{J_i J_{i+1}\} + 3t_4 \left( [\{\hat{\mathbf{k}}\delta\} \times \mathbf{n}] \cdot \mathbf{J} \right) \right], \\
H_{kn^2}^{S(\Gamma_{15})}(\hat{\mathbf{k}}, \mathbf{R}) &= \frac{\hbar^2}{2m_0} \left[ i2\sqrt{3}w_1 \sum_i [\hat{k}_i \delta] (\mathbf{n} \cdot \mathbf{n}) \{J_{i+1} J_{i+2}\} + \right. \\
&\quad i2\sqrt{3}w_2 \sum_i [\hat{k}_i \delta] (2n_i^2 - n_{i+1}^2 - n_{i+2}^2) \{J_{i+1} J_{i+2}\} + \\
&\quad 3w_3 \sum_i \left\{ \hat{k}_i \delta \right\} (n_{i+1}^2 - n_{i+2}^2) J_i + iw_4 ([\hat{\mathbf{k}}\delta] \cdot \mathbf{N}) I + \\
&\quad i6w_5 \sum_i \left( [\hat{k}_i \delta] N_i - \frac{1}{3} ([\hat{\mathbf{k}}\delta] \cdot \mathbf{N}) \right) J_i^2 + \\
&\quad \left. i12w_6 \sum_i \left\{ [\hat{k}_i \delta] N_{i+1} \right\} \{J_i J_{i+1}\} + 3w_7 ([\{\hat{\mathbf{k}}\delta\} \times \mathbf{N}] \cdot \mathbf{J}) \right].
\end{aligned}$$

Here  $I$  is a unit matrix  $3 \times 3$ ,  $J_i$  are matrices of the angular momentum  $J = 1$ .

#### A4. $\Gamma_8$ band Hamiltonian

$$H_{n^2}^{S(\Gamma_8)}(\mathbf{R}) = \frac{\hbar^2}{2m_0a_0} \left[ \xi_1 (\mathbf{n} \cdot \mathbf{n}) I \delta(\mathbf{nR}) + 2\xi_2 \sum_i (n_i^2 - \frac{1}{3}) J_i^2 \delta(\mathbf{nR}) + 4\xi_3 \sum_i N_i \{J_{i+1} J_{i+2}\} \delta(\mathbf{nR}) \right],$$

$$H_{kn}^{S(\Gamma_8)}(\hat{\mathbf{k}}, \mathbf{R}) = \frac{\hbar^2}{2m_0} \left[ i\tau_1 \left( [\hat{\mathbf{k}}\delta] \cdot \mathbf{n} \right) I + i2\tau_2 \sum_i \left( [\hat{k}_i\delta] n_i - \frac{1}{3} ([\hat{\mathbf{k}}\delta] \cdot \mathbf{n}) \right) J_i^2 + i4\tau_3 \sum_i \left\{ [\hat{k}_i\delta] n_{i+1} \right\} \{J_i J_{i+1}\} + 2\tau_4 \left( [\{\hat{\mathbf{k}}\delta\} \times \mathbf{n}] \cdot \mathbf{J} \right) + 8\tau_5 \sum_i \left\{ [\{\hat{\mathbf{k}}\delta\} \times \mathbf{n}]_i J_i^3 + \frac{4}{\sqrt{3}} \tau_6 \sum_i \left\{ \{\hat{k}_{i+1}\delta\} n_{i+2} \right\} \left\{ J_i (J_{i+1}^2 - J_{i+2}^2) \right\} \right] \right],$$

$$H_{kn^2}^{S(\Gamma_8)}(\hat{\mathbf{k}}, \mathbf{R}) = \frac{\hbar^2}{2m_0} \left[ i\frac{2}{\sqrt{3}}\chi_1 \sum_i [\hat{k}_i\delta] (\mathbf{n} \cdot \mathbf{n}) \{J_{i+1} J_{i+2}\} + i\frac{2}{\sqrt{3}}\chi_2 \sum_i [\hat{k}_i\delta] (2n_i^2 - n_{i+1}^2 - n_{i+2}^2) \{J_{i+1} J_{i+2}\} + 2\chi_3 \sum_i \{\hat{k}_i\delta\} (n_{i+1}^2 - n_{i+2}^2) J_i + i\chi_4 ([\hat{\mathbf{k}}\delta] \cdot \mathbf{N}) I + i2\chi_5 \sum_i \left( [\hat{k}_i\delta] N_i - \frac{1}{3} ([\hat{\mathbf{k}}\delta] \cdot \mathbf{N}) \right) J_i^2 + i4\chi_6 \sum_i \left\{ [\hat{k}_i\delta] N_{i+1} \right\} \{J_i J_{i+1}\} + 2\chi_7 \left( [\{\hat{\mathbf{k}}\delta\} \times \mathbf{N}] \cdot \mathbf{J} \right) + \frac{4}{\sqrt{3}}\chi_8 \sum_i \{\hat{k}_i\delta\} (\mathbf{n} \cdot \mathbf{n}) \left\{ J_i (J_{i+1}^2 - J_{i+2}^2) \right\} + \frac{4}{\sqrt{3}}\chi_9 \sum_i \{\hat{k}_i\delta\} (2n_i^2 - n_{i+1}^2 - n_{i+2}^2) \left\{ J_i (J_{i+1}^2 - J_{i+2}^2) \right\} + 8\chi_{10} \sum_i \{\hat{k}_i\delta\} (n_{i+1}^2 - n_{i+2}^2) J_i^3 + \frac{4}{\sqrt{3}}\chi_{11} \sum_i \left\{ \{\hat{k}_{i+1}\delta\} N_{i+2} \right\} \left\{ J_i (J_{i+1}^2 - J_{i+2}^2) \right\} + 8\chi_{12} \sum_i [\{\hat{\mathbf{k}}\delta\} \times \mathbf{N}]_i J_i^3 \right].$$

Here  $I$  is a unit matrix  $4 \times 4$ ,  $J_i$  are matrices of the angular momentum  $J = 3/2$ . If we neglect spin-orbit mixing  $\xi_i = s_i$  ( $i = 1, 2, 3$ ),  $\tau_i = t_i$  ( $i = 1, 2, 3, 4$ ),  $\chi_i = w_i$  ( $i = 1, \dots, 7$ ),  $\tau_5 = \tau_6 = \chi_8 = \dots = \chi_{12} = 0$ .

#### A5. $\Gamma_8 \oplus \Gamma_7$ band Hamiltonian

$$H_{\xi}^{S(\Gamma_8 \oplus \Gamma_7)}(\hat{\mathbf{k}}, \mathbf{R}) = \begin{bmatrix} H_{\xi}^{S(\Gamma_8)}(\hat{\mathbf{k}}, \mathbf{R}) & H_{\xi}^{S(\Gamma_8 \Gamma_7)}(\hat{\mathbf{k}}, \mathbf{R}) \\ H_{\xi}^{S(\Gamma_8 \Gamma_7)^+}(\hat{\mathbf{k}}, \mathbf{R}) & H_{\xi}^{S(\Gamma_7)}(\hat{\mathbf{k}}, \mathbf{R}) \end{bmatrix},$$

Here  $\xi = n^2, kn, kn^2$ ;  $H_{\xi}^{S(\Gamma_8)}(\hat{\mathbf{k}}, \mathbf{R})$  coincide with the corresponding matrices of the  $\Gamma_8$  band (see Appendix A4), in which  $\tau_5 = \tau_6 = \chi_8 = \dots = \chi_{12} = 0$ .

$$H_{n^2}^{S(\Gamma_7)}(\mathbf{R}) = \frac{\hbar^2}{2m_0 a_0} \xi_1 (\mathbf{n} \cdot \mathbf{n}) I \delta(\mathbf{nR}),$$

$$H_{kn}^{S(\Gamma_7)}(\hat{\mathbf{k}}, \mathbf{R}) = \frac{\hbar^2}{2m_0} \left[ i\tau_1 \left( [\hat{\mathbf{k}}\delta] \cdot \mathbf{n} \right) I + 2\tau_4 \left( [\{\hat{\mathbf{k}}\delta\} \times \mathbf{n}] \cdot \sigma \right) \right],$$

$$H_{kn^2}^{S(\Gamma_7)}(\hat{\mathbf{k}}, \mathbf{R}) = \frac{\hbar^2}{2m_0} \left[ 2\chi_3 \sum_i \{\hat{k}_i \delta\} (n_{i+1}^2 - n_{i+2}^2) \sigma_i + \right. \\ \left. i\chi_4 \left( [\hat{\mathbf{k}}\delta] \cdot \mathbf{N} \right) I + 2\chi_7 \left( [\{\hat{\mathbf{k}}\delta\} \times \mathbf{N}] \cdot \sigma \right) \right],$$

$$H_{n^2}^{S(\Gamma_8 \Gamma_7)}(\mathbf{R}) = \frac{\hbar^2}{2m_0 a_0} \left[ \sqrt{2}\xi_2 \left[ (2n_z^2 - n_x^2 - n_y^2) I_1^{\Gamma_{12}} + \sqrt{3}(n_x^2 - n_y^2) I_2^{\Gamma_{12}} \right] \delta(\mathbf{nR}) + \right. \\ \left. \sqrt{6}\xi_3 \sum_i N_i I_i^{\Gamma_{15}} \delta(\mathbf{nR}) \right],$$

$$H_{kn}^{S(\Gamma_8 \Gamma_7)}(\hat{\mathbf{k}}, \mathbf{R}) = \frac{\hbar^2}{2m_0} \left[ i\sqrt{2}\tau_2 \left[ (2[\hat{k}_z \delta] n_z - [\hat{k}_x \delta] n_x - [\hat{k}_y \delta] n_y) I_1^{\Gamma_{12}} + \sqrt{3}([\hat{k}_x \delta] n_x - [\hat{k}_y \delta] n_y) I_2^{\Gamma_{12}} \right] + \right. \\ \left. i\sqrt{6}\tau_3 \sum_i \{[\hat{k}_{i+1} \delta] n_{i+2}\} I_i^{\Gamma_{15}} + \frac{1}{\sqrt{2}}\tau_4 \sum_i [\{\hat{\mathbf{k}}\delta\} \times \mathbf{n}]_i I_i^{\Gamma_{25}} \right],$$

$$H_{kn^2}^{S(\Gamma_8 \Gamma_7)}(\hat{\mathbf{k}}, \mathbf{R}) = \frac{\hbar^2}{2m_0} \left[ i\frac{1}{\sqrt{2}}\chi_1 \sum_i [\hat{k}_i \delta] (\mathbf{n} \cdot \mathbf{n}) I_i^{\Gamma_{15}} + \right. \\ i\frac{1}{\sqrt{2}}\chi_2 \sum_i [\hat{k}_i \delta] (2n_i^2 - n_{i+1}^2 - n_{i+2}^2) I_i^{\Gamma_{15}} + \frac{1}{\sqrt{2}}\chi_3 \sum_i \{\hat{k}_i \delta\} (n_{i+1}^2 - n_{i+2}^2) I_i^{\Gamma_{25}} + \\ i\sqrt{2}\chi_5 \left[ (2[\hat{k}_z \delta] N_z - [\hat{k}_x \delta] N_x - [\hat{k}_y \delta] N_y) I_1^{\Gamma_{12}} + \sqrt{3}([\hat{k}_x \delta] N_x - [\hat{k}_y \delta] N_y) I_2^{\Gamma_{12}} \right] + \\ \left. i\sqrt{6}\chi_6 \sum_i \{[\hat{k}_{i+1} \delta] N_{i+2}\} I_i^{\Gamma_{15}} + \frac{1}{\sqrt{2}}\chi_7 \sum_i [\{\hat{\mathbf{k}}\delta\} \times \mathbf{N}]_i I_i^{\Gamma_{25}} \right].$$

## APPENDIX B: MATRICES $I_i^{\Gamma_\alpha}$

Matrices  $I_i^{\Gamma_\alpha}$ , used to obtain the  $H^{(\Gamma_8 \Gamma_7)}(\hat{\mathbf{k}}, \mathbf{R})$  block of the  $\Gamma_8 \oplus \Gamma_7$  two-band Hamiltonian are:

$$I_1^{\Gamma_{12}} = \begin{bmatrix} 0 & 0 \\ -1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix};$$



$$I_2^{\Gamma_{12}} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ -1 & 0 \end{bmatrix};$$

$$I_x^{\Gamma_{15}} = \begin{bmatrix} -i & 0 \\ 0 & i\sqrt{3} \\ -i\sqrt{3} & 0 \\ 0 & i \end{bmatrix};$$

$$I_y^{\Gamma_{15}} = \begin{bmatrix} 1 & 0 \\ 0 & -\sqrt{3} \\ -\sqrt{3} & 0 \\ 0 & 1 \end{bmatrix};$$

$$I_z^{\Gamma_{15}} = \begin{bmatrix} 0 & -i2 \\ 0 & 0 \\ 0 & 0 \\ -i2 & 0 \end{bmatrix};$$

$$I_x^{\Gamma_{25}} = \begin{bmatrix} \sqrt{3} & 0 \\ 0 & 1 \\ -1 & 0 \\ 0 & -\sqrt{3} \end{bmatrix};$$

$$I_y^{\Gamma_{25}} = \begin{bmatrix} -i\sqrt{3} & 0 \\ 0 & -i \\ -i & 0 \\ 0 & -i\sqrt{3} \end{bmatrix};$$

$$I_z^{\Gamma_{25}} = \begin{bmatrix} 0 & 0 \\ -2 & 0 \\ 0 & -2 \\ 0 & 0 \end{bmatrix};$$

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